Semiconductors

Why can we ignore e-e interactions?

With interactions, the energy would depend not just on whether a state is occupied or not, it would also depend on whether the other states are occupied.

Phonon calculation

1. Write down the classical equations of motion.
2. Linearize the equations
3. The solutions of the linear equations or eigenfunctions of the translation operator. They decouple into normal modes.
4. Quantize the normal modes separately.

Landau theory of a Fermi liquid

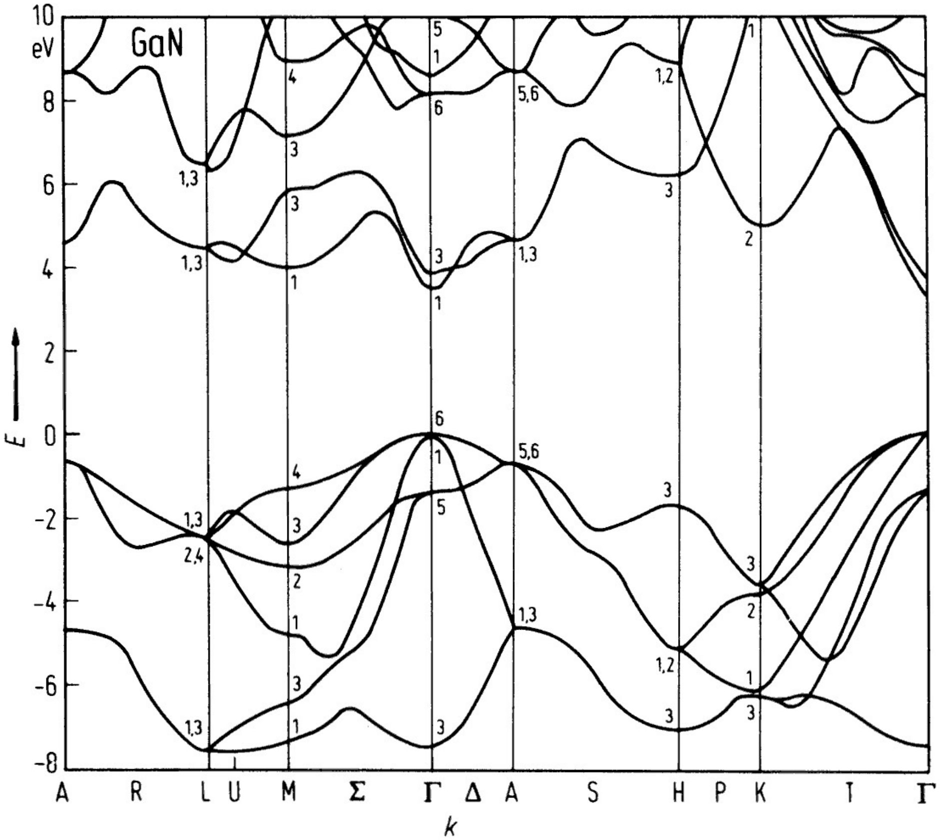
Landau first considered small displacements of the electrons from the many-electron ground state. The "normal modes" of this interacting electron system. The low lying excitations he called quasiparticles.

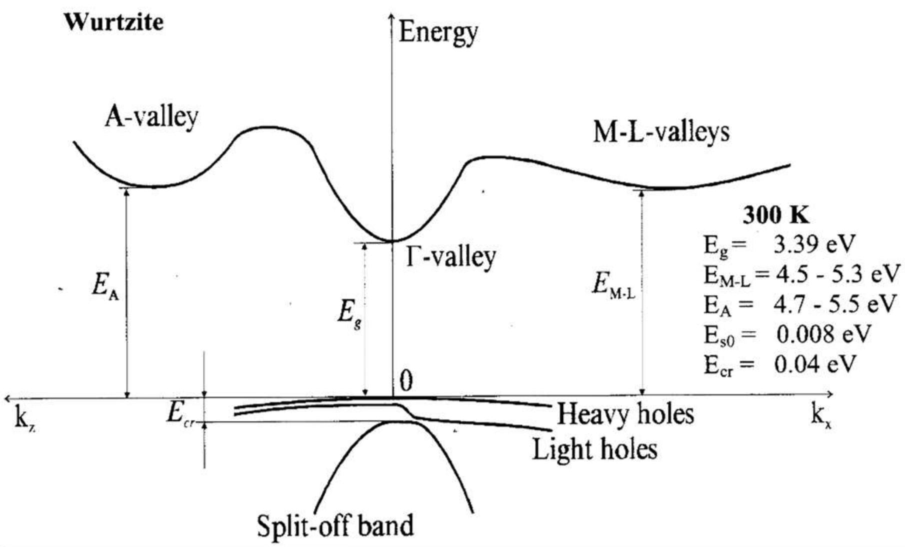
The quasiparticles have as many degrees of freedom as the electrons. They can be labeled by k.

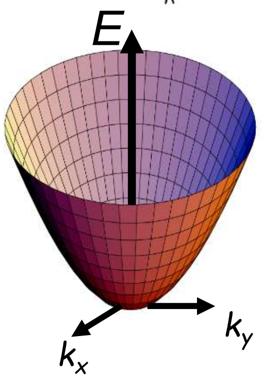
Quasiparticles can be have the same spin, charge, and k vectors as the electrons.

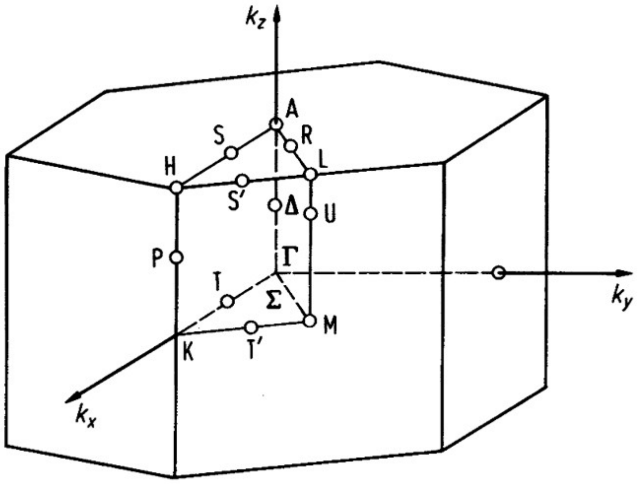
Concepts like the density of states refer to quasiparticles.

GaN









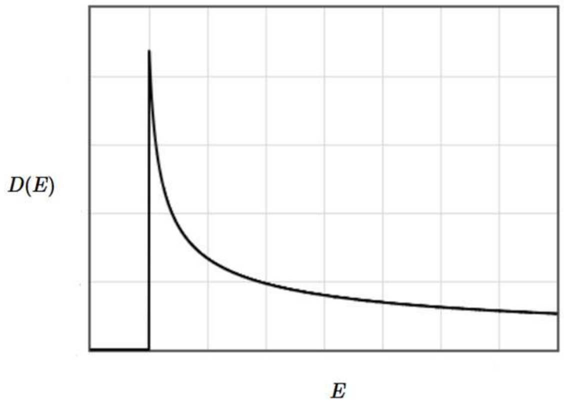
1st Brillioun zone of hcp

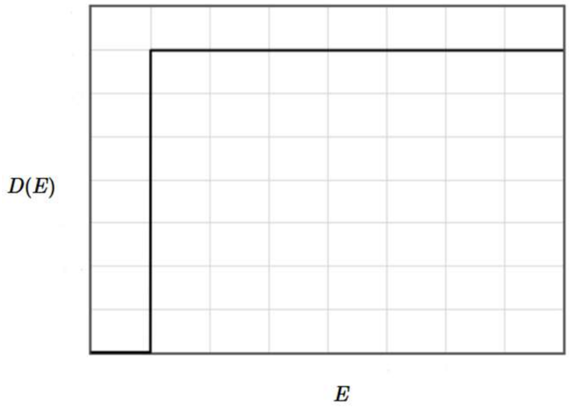
Free electron Fermi gas

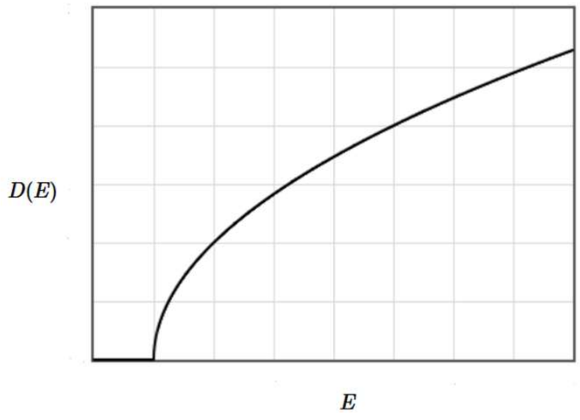
1 - d $$D(E) = \sqrt{\frac{2m}{\hbar^2 \pi^2 E}} = \frac{n}{2\sqrt{E_F E}} \quad \mathrm{J^{-1}m^{-1}}$$

2 - d $$D(E) = \frac{m}{\hbar^2 \pi} = \frac{n}{E_F} \quad \mathrm{J^{-1}m^{-2}}$$

3 - d $$D(E) = \frac{\pi}{2}\left(\frac{2m}{\hbar^2 \pi^2}\right)^{3/2}\sqrt{E} = \frac{3n}{2E_F^{3/2}}\sqrt{E} \quad \mathrm{J^{-1}m^{-3}}$$







Measuring the effective mass

Cyclotron resonance $\omega_c = \frac{eB}{m^*}$

Resonant absorption occurs when rf waves with the cyclotron resonance frequency are applied. This can be used to experimentally determine the effective mass.

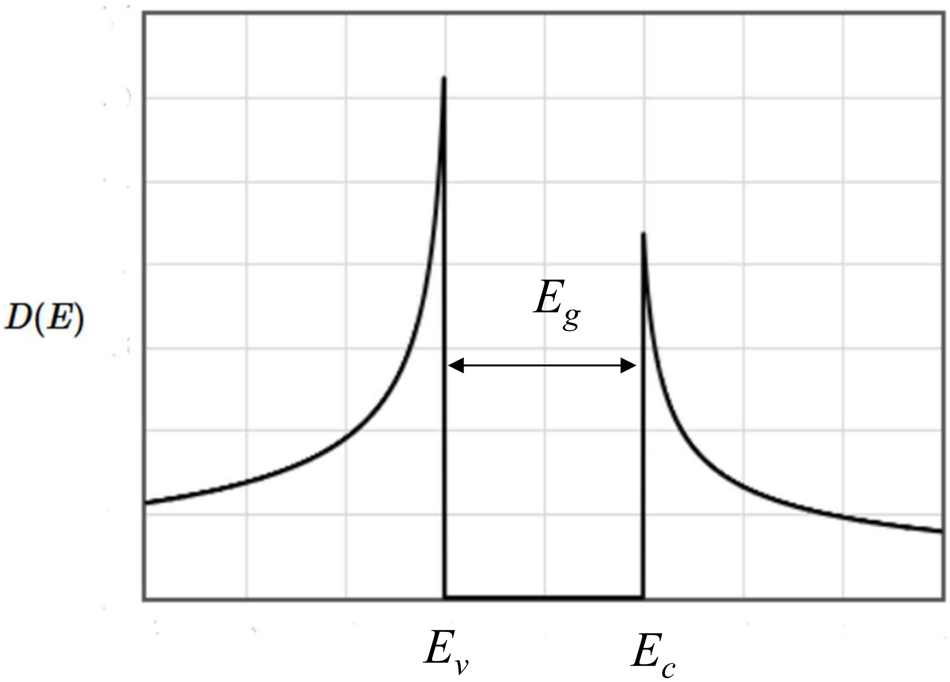
Knowing the effective mass, the scattering time can be calculated from the measured conductivity.

$$\sigma = \frac{ne^2\tau_{sc}}{m^*}$$

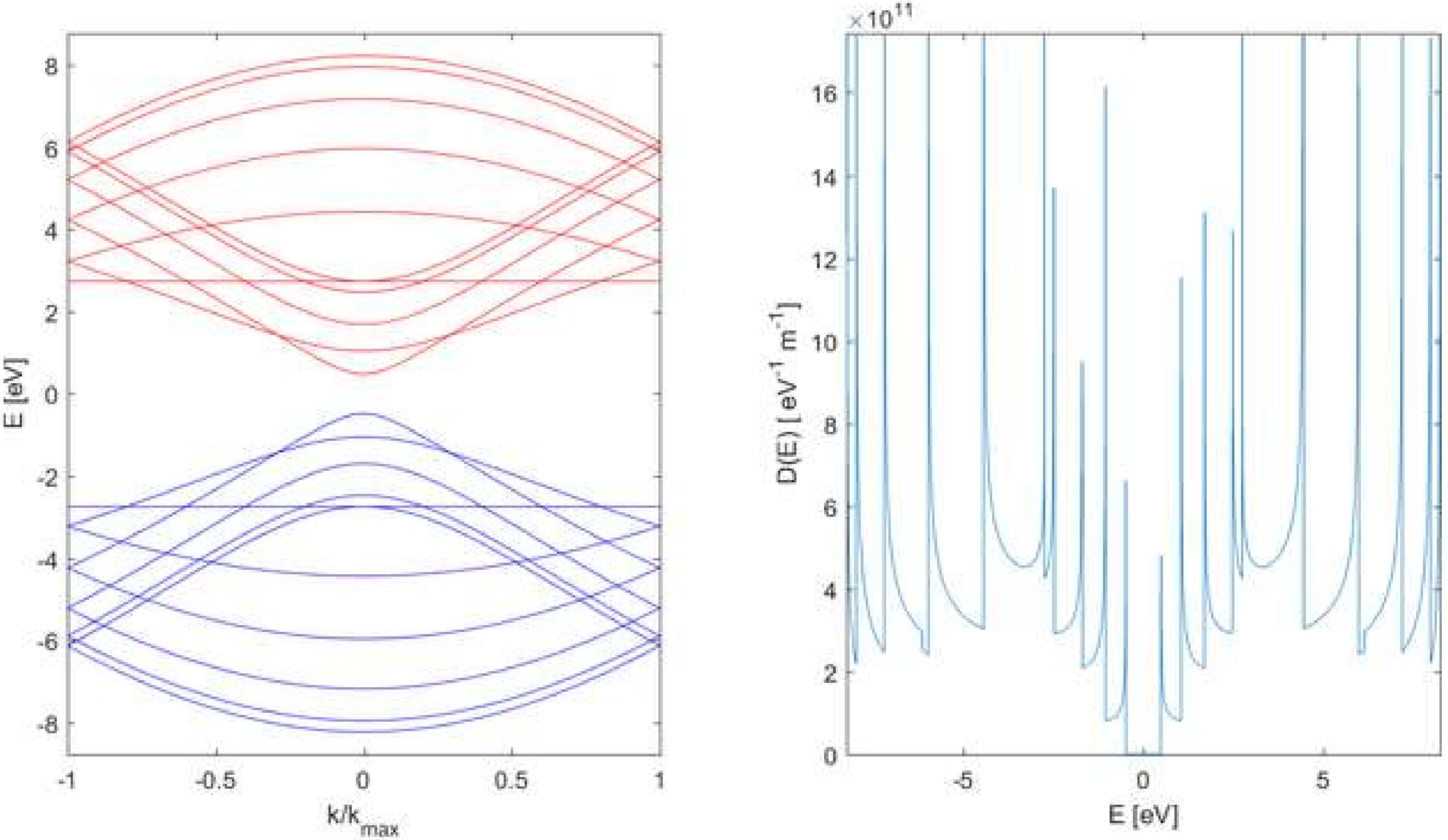
Semiconductors and insulators - 1d

$$E = \frac{\hbar^2 (\vec{k} - \vec{k}_0)^2}{2m^*}$$

$$D(E) = \begin{cases} \dfrac{D_c}{\sqrt{(E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ \dfrac{D_v}{\sqrt{(E - E_c)}} & E_c < E \end{cases} \quad \text{J}^{-1}\text{m}^{-3}$$

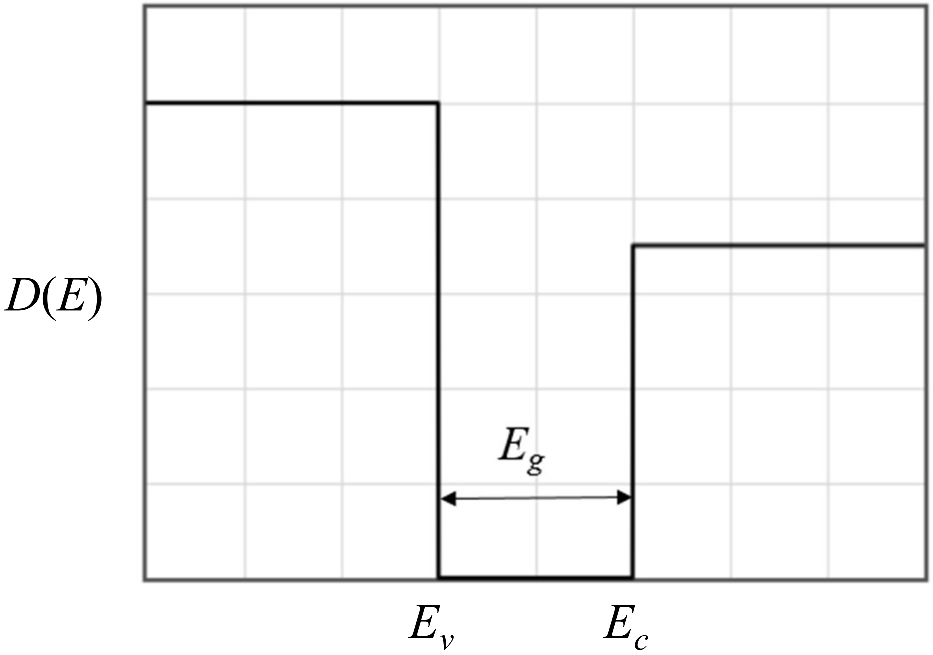


Semiconducting carbon nanotubes



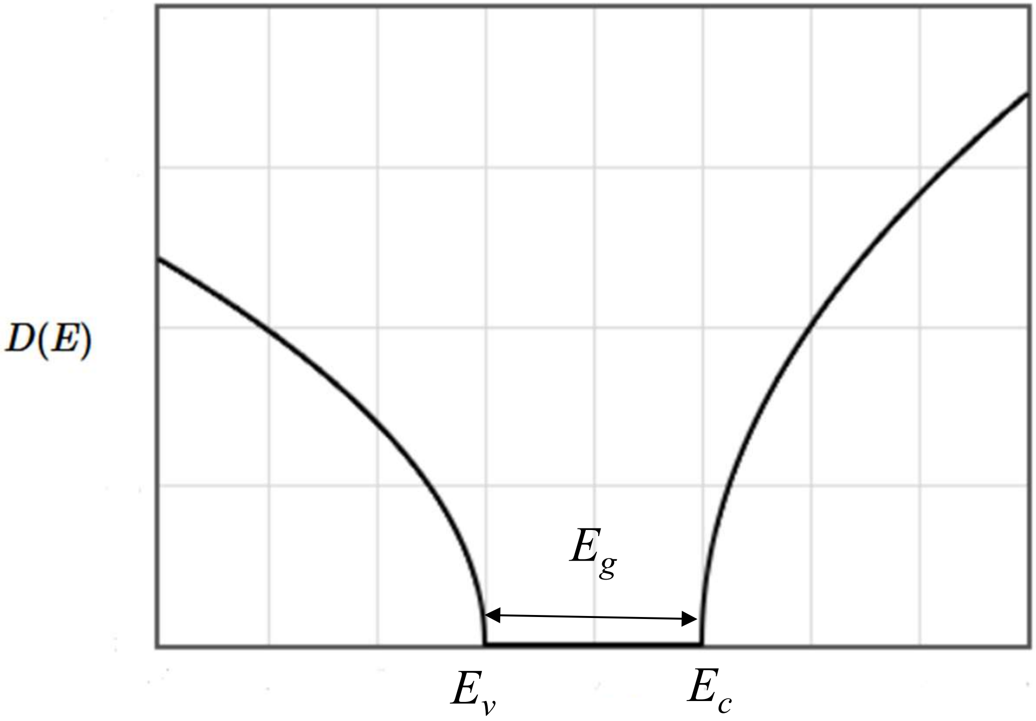
Semiconductors and insulators - 2d

$$D(E) = \begin{cases} D_c & E < E_v \\ 0 & E_v < E < E_c \\ D_v & E_c < E \end{cases} \quad \mathrm{J^{-1}m^{-3}}$$

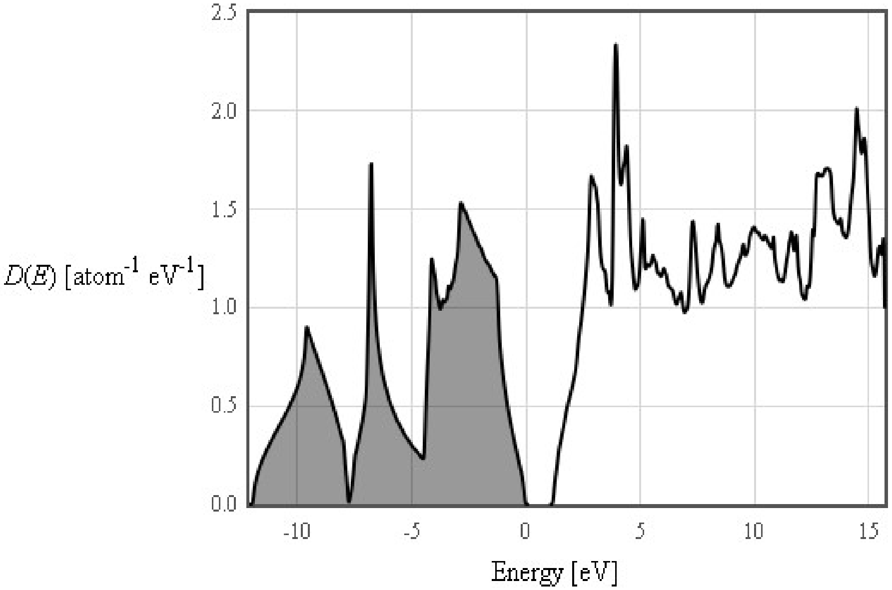


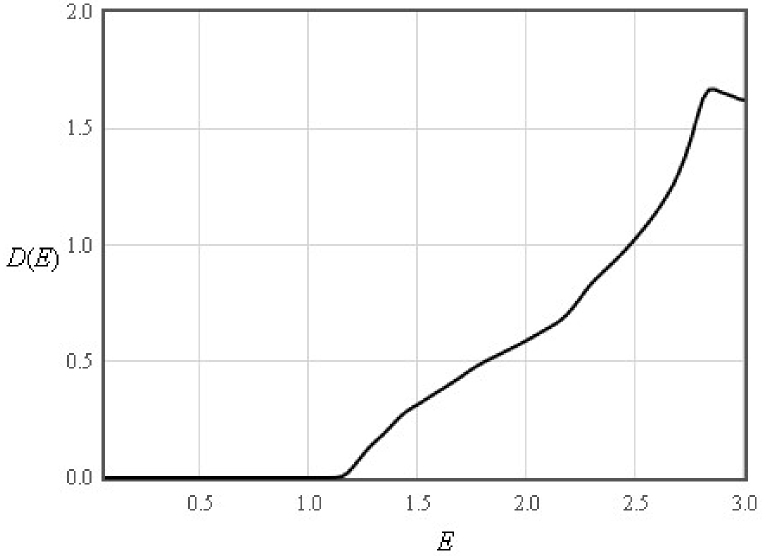
Semiconductors and insulators - 3d

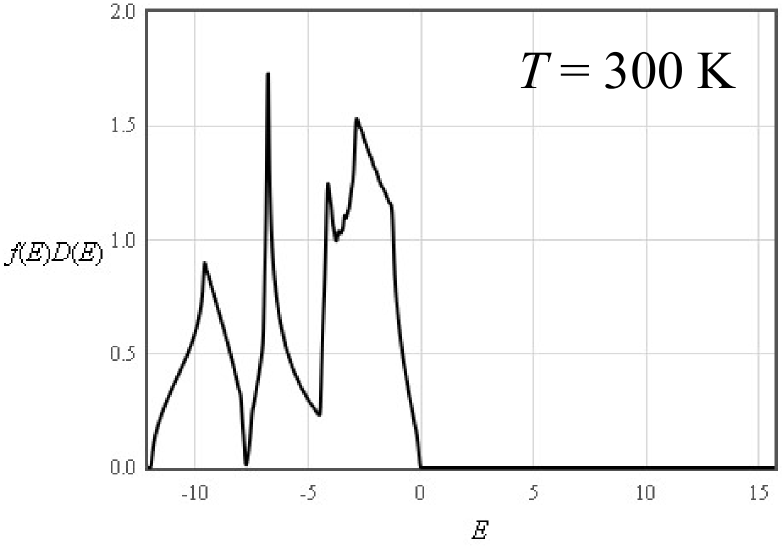
$$D(E) = \begin{cases} D_c\sqrt{E_v - E} & E < E_v \\ 0 & E_v < E < E_c \\ D_v\sqrt{E - E_c} & E_c < E \end{cases} \quad \mathrm{J^{-1}m^{-3}}$$

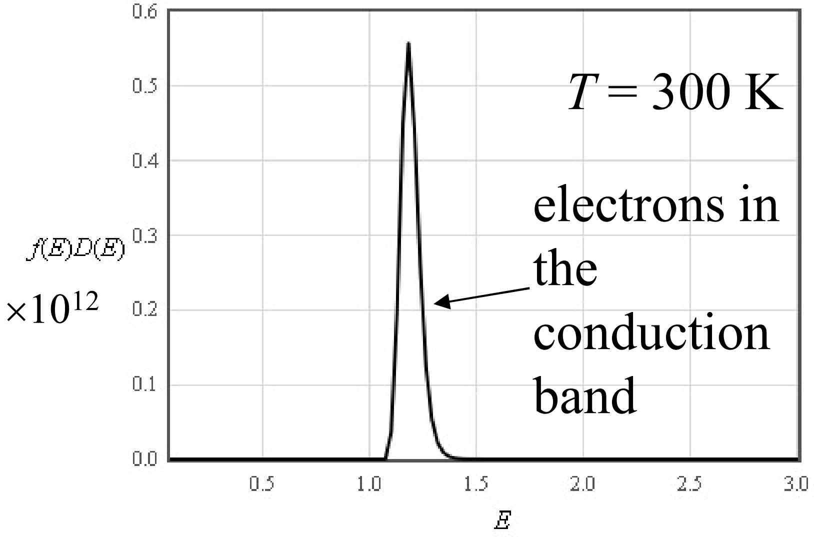


Silicon density of states






T = 300 K


T = 300 K

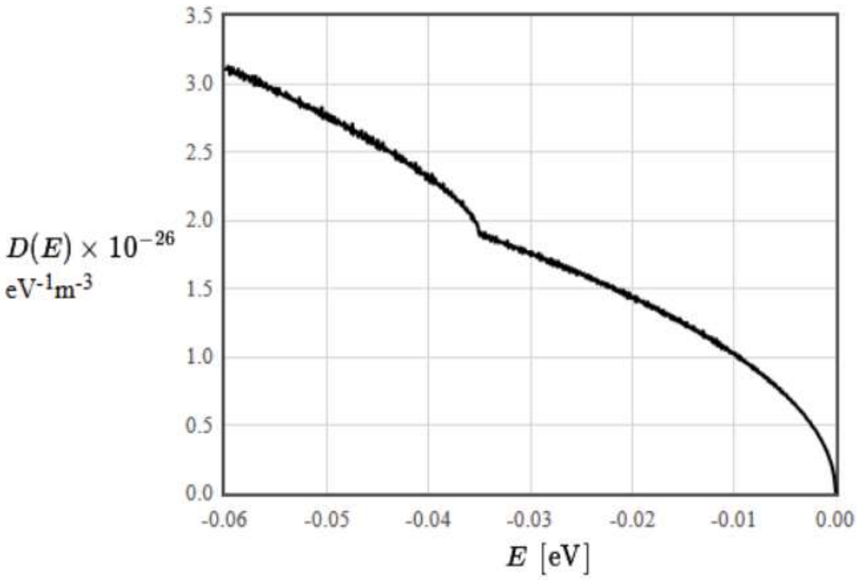
electrons in the conduction band

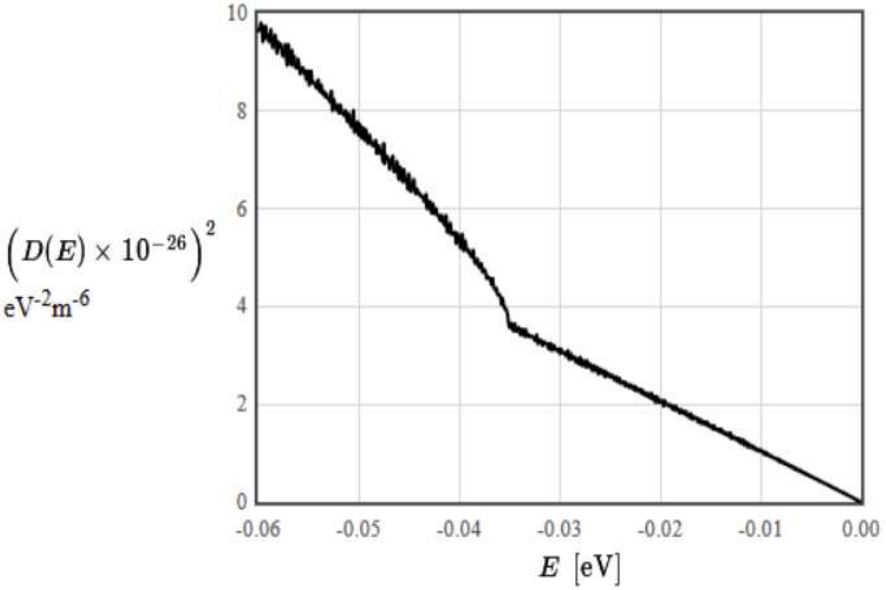
Silicon valence bands

$$E_{v,lh} = -\frac{\hbar^2}{2m_e}\left(4.1k^2 - \sqrt{1.21k^4 + 4.1(k_x^2k_y^2 + k_x^2k_z^2 + k_y^2k_z^2)}\right),$$

$$E_{v,hh} = -\frac{\hbar^2}{2m_e}\left(4.1k^2 + \sqrt{1.21k^4 + 4.1(k_x^2k_y^2 + k_x^2k_z^2 + k_y^2k_z^2)}\right),$$

$$E_{v,so} = -E_{so} - \frac{\hbar^2 k^2}{2m_{so}}.$$





Boltzmann Approximation

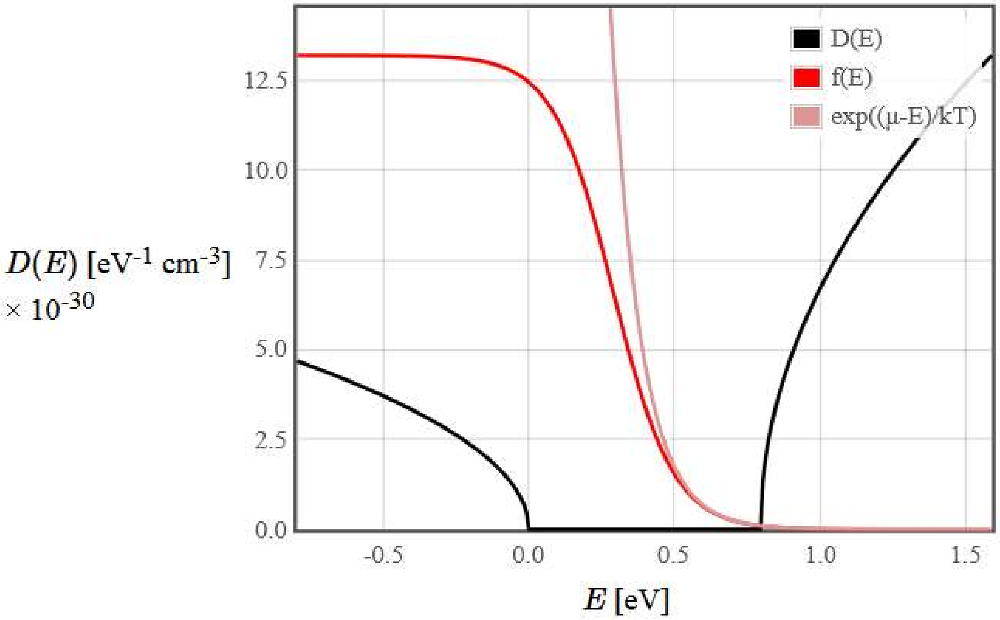
Density of electrons in the conduction band

The free electron density of states is modified by the effective mass.

$$D(E) = D_c\sqrt{E - E_c}$$

$$f(E) = \frac{1}{1 + \exp\left(\frac{E - \mu}{k_B T}\right)} \approx \exp\left(\frac{\mu - E}{k_B T}\right)$$

Boltzmann
approximation
$E_c - \mu > 3k_BT$



$$n = \int_{E_c}^{\infty} D(E) f(E)\, dE \approx D_c \int_{E_c}^{\infty} \exp\left(\frac{\mu - E}{k_B T}\right)\sqrt{E - E_c}\, dE$$

Density of electrons in the conduction band

$$n = \int_{E_c}^{\infty} D(E) f(E) dE \approx D_c \int_{E_c}^{\infty} \exp\left(\frac{\mu - E}{k_B T}\right) \sqrt{E - E_c}\, dE$$

$$= D_c \exp\left(\frac{\mu - E_c}{k_B T}\right) \int_{E_c}^{\infty} \exp\left(-\frac{E - E_c}{k_B T}\right) \sqrt{E - E_c}\, dE$$

$$x = E - E_c \qquad \int_0^{\infty} \sqrt{x} \exp\left(\frac{-x}{k_B T}\right) dx = \frac{2}{\sqrt{\pi}} (k_B T)^{3/2}$$

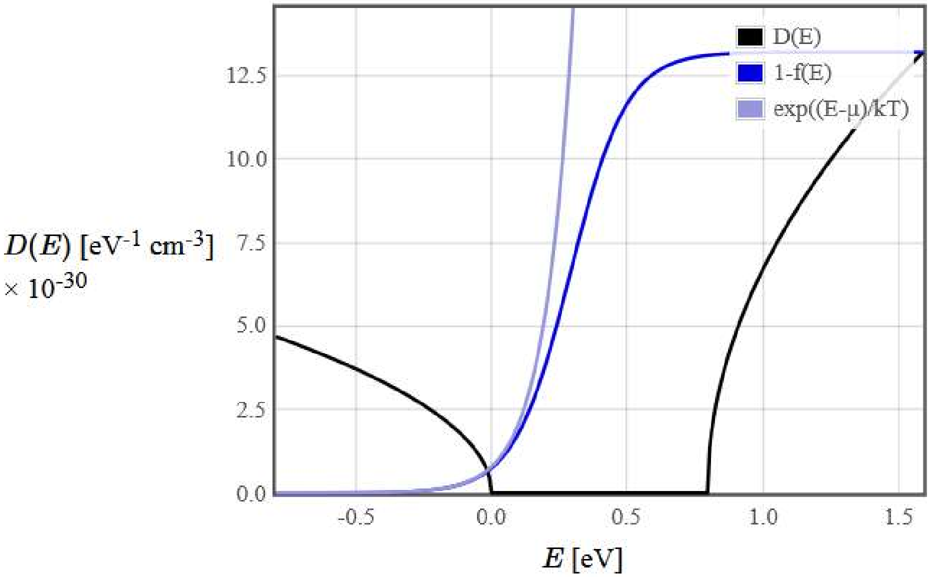
$$\boxed{n = N_c(T) \exp\left(\frac{\mu - E_c}{k_B T}\right)} = \frac{2D_c}{\sqrt{\pi}} (k_B T)^{3/2} \exp\left(\frac{\mu - E_c}{k_B T}\right)$$

$$N_c = \frac{2D_c}{\sqrt{\pi}} (k_B T)^{3/2} = 2\left(\frac{m^* k_B T}{2\pi\hbar^2}\right)^{3/2} = \text{effective density of states}$$

Density of holes in the valence band

$$D(E) = D_v \sqrt{E_v - E}$$

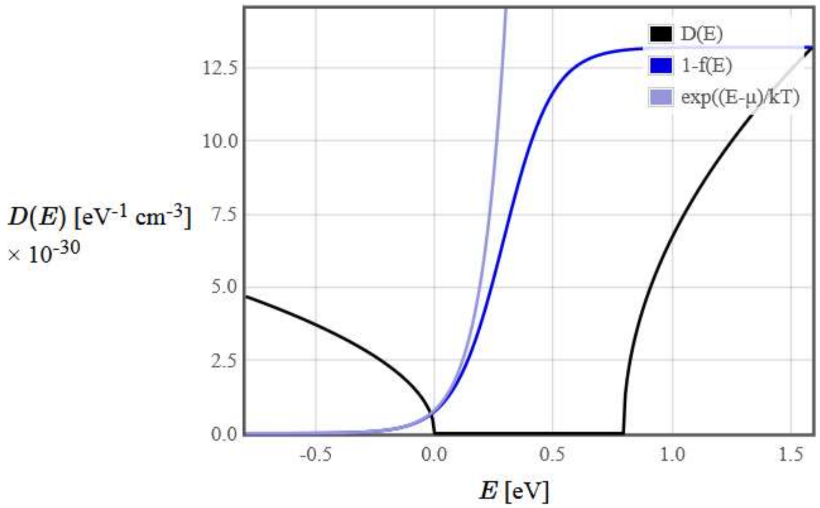
$$1 - f(E) = 1 - \frac{1}{1 + \exp\left(\frac{E-\mu}{k_B T}\right)} \approx \exp\left(\frac{E-\mu}{k_B T}\right)$$



Boltzmann approximation
$\mu - E_v > 3k_B T$

$$p = \int_{-\infty}^{E_v} D(E)\big(1 - f(E)\big)\,dE \approx D_v \int_{-\infty}^{E_v} \exp\left(\frac{E-\mu}{k_B T}\right)\sqrt{E_v - E}\,dE$$

Density of holes in the valence band



$$p = \int_{-\infty}^{E_v} D(E)\left(1-f(E)\right)dE \approx D_v \int_{-\infty}^{E_v} \exp\left(\frac{E-\mu}{k_BT}\right)\sqrt{E_v - E}\,dE$$

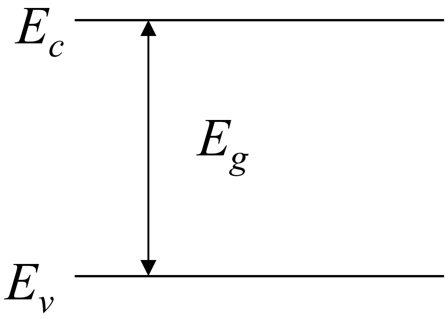
$$\boxed{p = N_v \exp\left(\frac{E_v-\mu}{k_BT}\right)} = \frac{2D_v}{\sqrt{\pi}}\left(k_BT\right)^{3/2}\exp\left(\frac{E_v-\mu}{k_BT}\right)$$

$$N_v = 2\left(\frac{m_h^* k_B T}{2\pi\hbar^2}\right)^{3/2}$$

= Effective density of states in the valence band

Law of mass action

$$np = N_c \exp\left(\frac{\mu - E_c}{k_B T}\right) N_v \exp\left(\frac{E_v - \mu}{k_B T}\right)$$



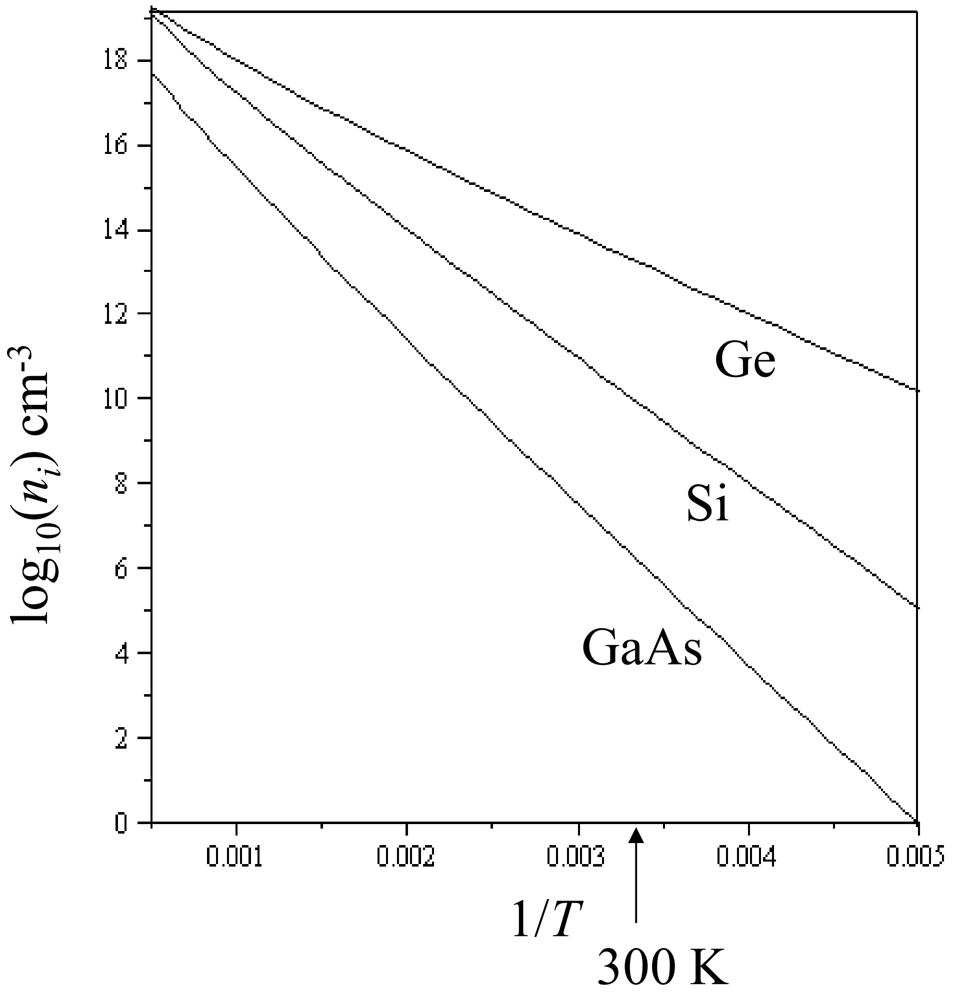
$$np = N_c N_v \exp\left(\frac{-E_g}{k_B T}\right)$$

For intrinsic semiconductors (no impurities)

$$\boxed{n = p = n_i = \sqrt{N_c N_v} \exp\left(\frac{-E_g}{2k_B T}\right)}$$

intrinsic carrier density

Intrinsic carrier concentration



$$n_i = \sqrt{N_v N_c \left(\frac{T}{300}\right)^3} \exp\left(-\frac{E_g}{2k_B T}\right)$$

~ 5 x 10^{22} atoms/cm^3

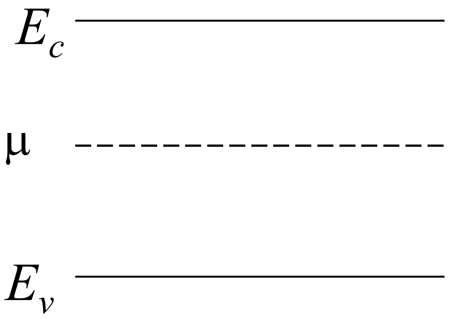
Chemical potential of an intrinsic semiconductor

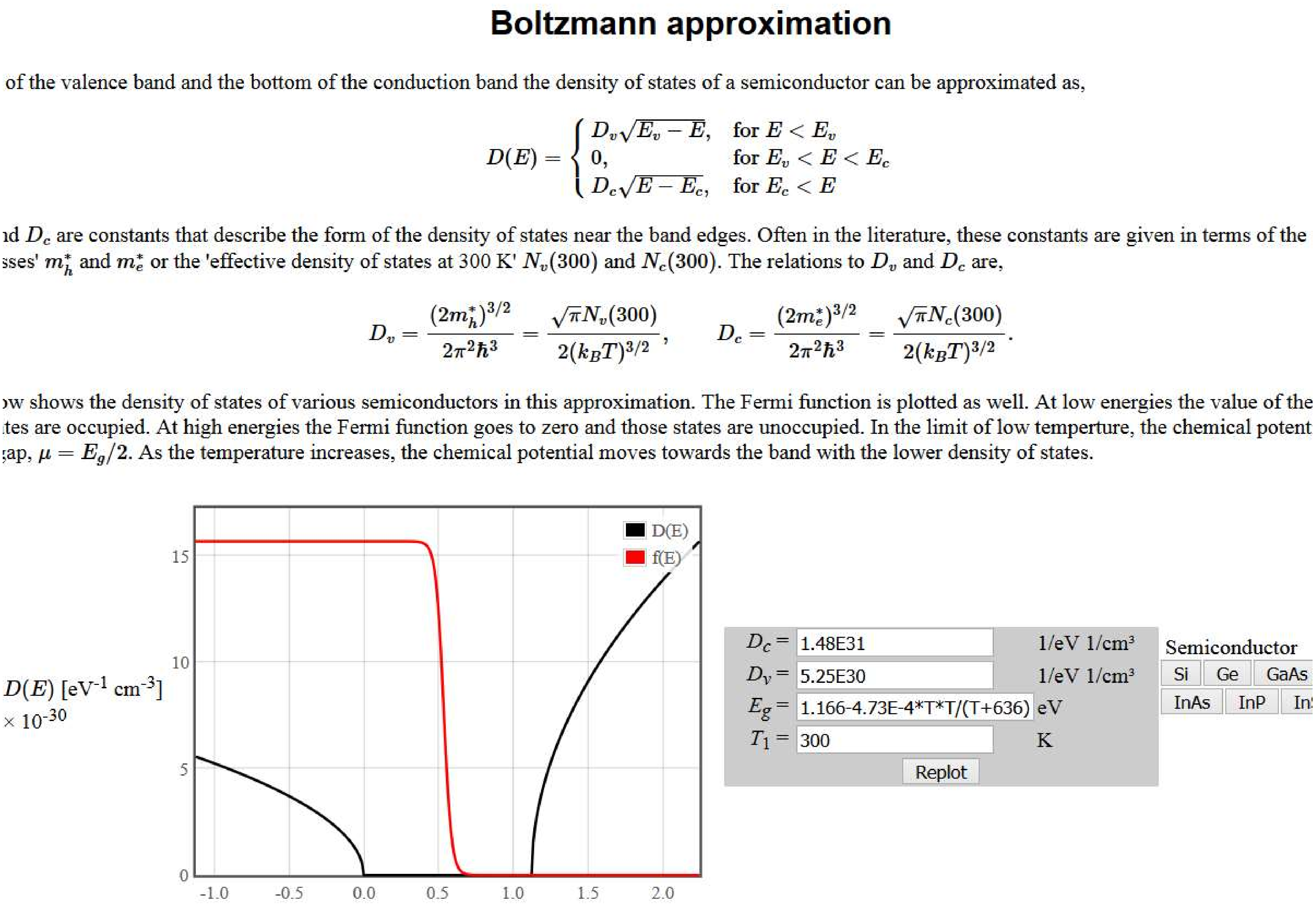
$$n = p = N_c \exp\left(\frac{\mu - E_c}{k_B T}\right) = N_v \exp\left(\frac{E_v - \mu}{k_B T}\right)$$

$$\exp\left(\frac{\mu - E_c - E_v + \mu}{k_B T}\right) = \frac{N_v}{N_c}$$

$$\frac{2\mu}{k_B T} = \frac{E_c + E_v}{k_B T} + \ln\left(\frac{N_v}{N_c}\right)$$

$$\boxed{\mu = \frac{E_c + E_v}{2} + \frac{k_B T}{2}\ln\left(\frac{N_v}{N_c}\right)}$$





Boltzmann approximation

of the valence band and the bottom of the conduction band the density of states of a semiconductor can be approximated as,

$$D(E) = \begin{cases} D_v\sqrt{E_v - E}, & \text{for } E < E_v \\ 0, & \text{for } E_v < E < E_c \\ D_c\sqrt{E - E_c}, & \text{for } E_c < E \end{cases}$$

d D_c are constants that describe the form of the density of states near the band edges. Often in the literature, these constants are given in terms of the
sses' m_h^* and m_e^* or the 'effective density of states at 300 K' $N_v(300)$ and $N_c(300)$. The relations to D_v and D_c are,

$$D_v = \frac{(2m_h^*)^{3/2}}{2\pi^2\hbar^3} = \frac{\sqrt{\pi}N_v(300)}{2(k_BT)^{3/2}}, \qquad D_c = \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3} = \frac{\sqrt{\pi}N_c(300)}{2(k_BT)^{3/2}}.$$

w shows the density of states of various semiconductors in this approximation. The Fermi function is plotted as well. At low energies the value of the
tes are occupied. At high energies the Fermi function goes to zero and those states are unoccupied. In the limit of low temperture, the chemical potent
ap, $\mu = E_g/2$. As the temperature increases, the chemical potential moves towards the band with the lower density of states.

D_c = 1.48E31 1/eV 1/cm³

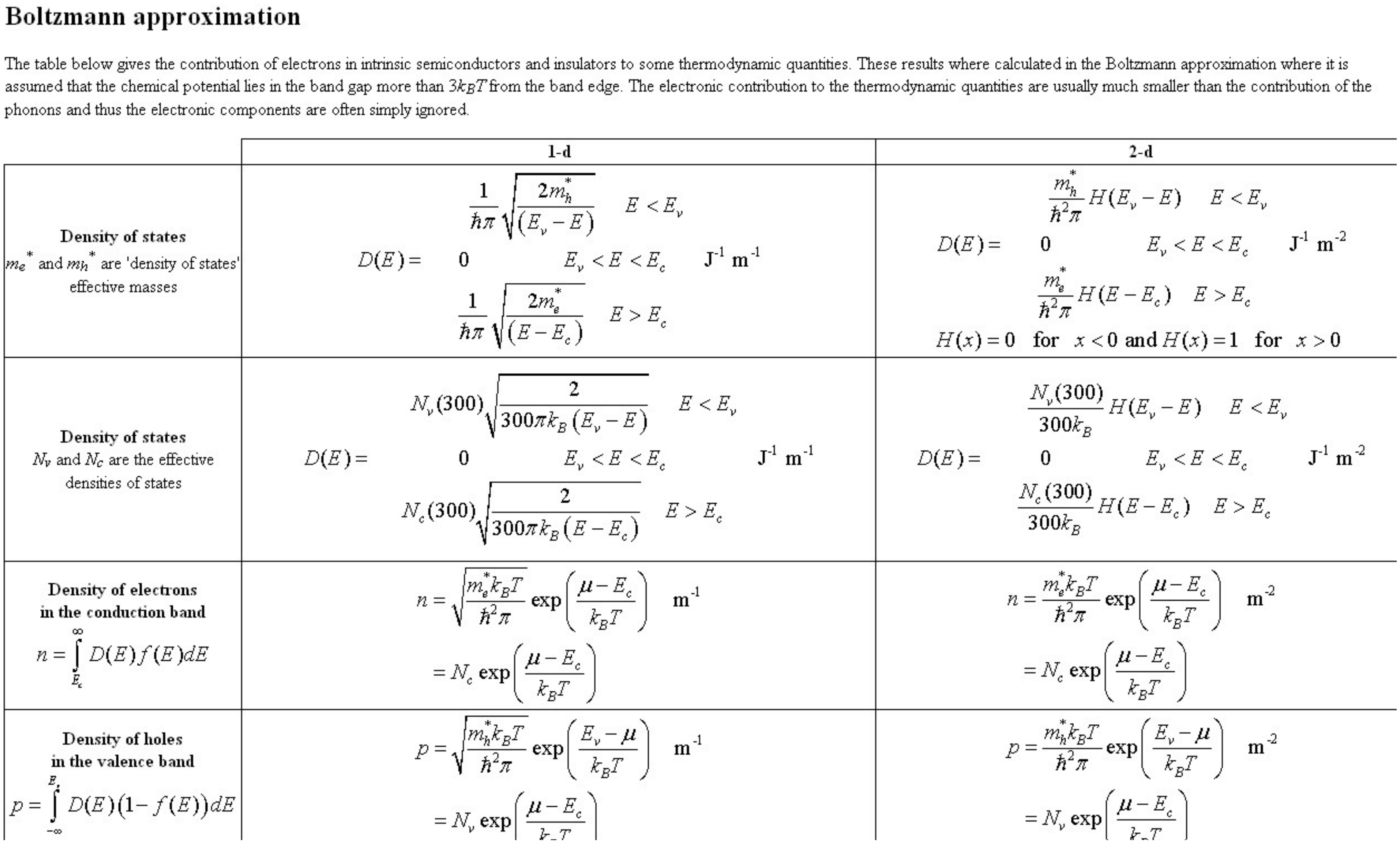
D_v = 5.25E30 1/eV 1/cm³

E_g = 1.166-4.73E-4*T*T/(T+636) eV

T_1 = 300 K

http://lampx.tugraz.at/~hadley/ss1/semiconductors/boltzmann.php

The electrical contribution to the thermodynamic properties of insulators depend on band edges



Boltzmann approximation

The table below gives the contribution of electrons in intrinsic semiconductors and insulators to some thermodynamic quantities. These results where calculated in the Boltzmann approximation where it is assumed that the chemical potential lies in the band gap more than $3k_BT$ from the band edge. The electronic contribution to the thermodynamic quantities are usually much smaller than the contribution of the phonons and thus the electronic components are often simply ignored.

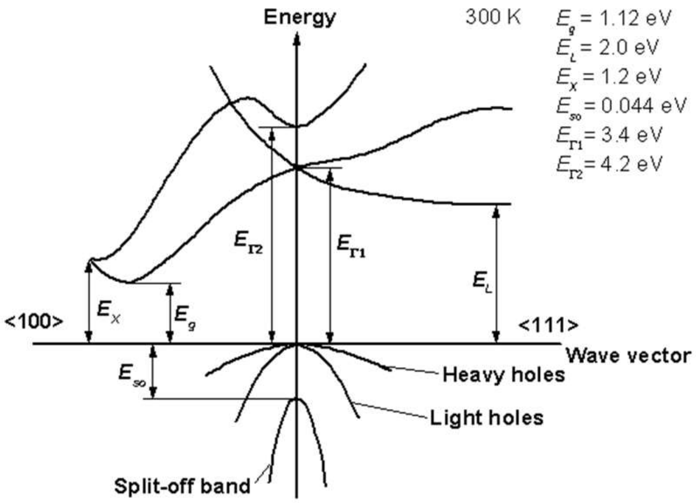
	1-d	**2-d**
Density of states m_e^* and m_h^* are 'density of states' effective masses	$D(E) = \begin{cases} \frac{1}{\hbar\pi}\sqrt{\frac{2m_h^*}{(E_v-E)}} & E<E_v \\ 0 & E_v<E<E_c \\ \frac{1}{\hbar\pi}\sqrt{\frac{2m_e^*}{(E-E_c)}} & E>E_c \end{cases}$ J^{-1} m^{-1}	$D(E) = \begin{cases} \frac{m_h^*}{\hbar^2\pi}H(E_v-E) & E<E_v \\ 0 & E_v<E<E_c \\ \frac{m_e^*}{\hbar^2\pi}H(E-E_c) & E>E_c \end{cases}$ J^{-1} m^{-2} $H(x)=0$ for $x<0$ and $H(x)=1$ for $x>0$
Density of states N_v and N_c are the effective densities of states	$D(E) = \begin{cases} N_v(300)\sqrt{\frac{2}{300\pi k_B(E_v-E)}} & E<E_v \\ 0 & E_v<E<E_c \\ N_c(300)\sqrt{\frac{2}{300\pi k_B(E-E_c)}} & E>E_c \end{cases}$ J^{-1} m^{-1}	$D(E) = \begin{cases} \frac{N_v(300)}{300k_B}H(E_v-E) & E<E_v \\ 0 & E_v<E<E_c \\ \frac{N_c(300)}{300k_B}H(E-E_c) & E>E_c \end{cases}$ J^{-1} m^{-2}
Density of electrons in the conduction band $n=\int_{E_c}^{\infty}D(E)f(E)dE$	$n=\sqrt{\frac{m_e^*k_BT}{\hbar^2\pi}}\exp\left(\frac{\mu-E_c}{k_BT}\right)$ m^{-1} $=N_c\exp\left(\frac{\mu-E_c}{k_BT}\right)$	$n=\frac{m_e^*k_BT}{\hbar^2\pi}\exp\left(\frac{\mu-E_c}{k_BT}\right)$ m^{-2} $=N_c\exp\left(\frac{\mu-E_c}{k_BT}\right)$
Density of holes in the valence band $p=\int_{-\infty}^{E_v}D(E)\left(1-f(E)\right)dE$	$p=\sqrt{\frac{m_h^*k_BT}{\hbar^2\pi}}\exp\left(\frac{E_v-\mu}{k_BT}\right)$ m^{-1} $=N_v\exp\left(\frac{\mu-E_c}{k_BT}\right)$	$p=\frac{m_h^*k_BT}{\hbar^2\pi}\exp\left(\frac{E_v-\mu}{k_BT}\right)$ m^{-2} $=N_v\exp\left(\frac{\mu-E_c}{k_BT}\right)$

New Semiconductor Materials. Biology systems.
Characteristics and Properties

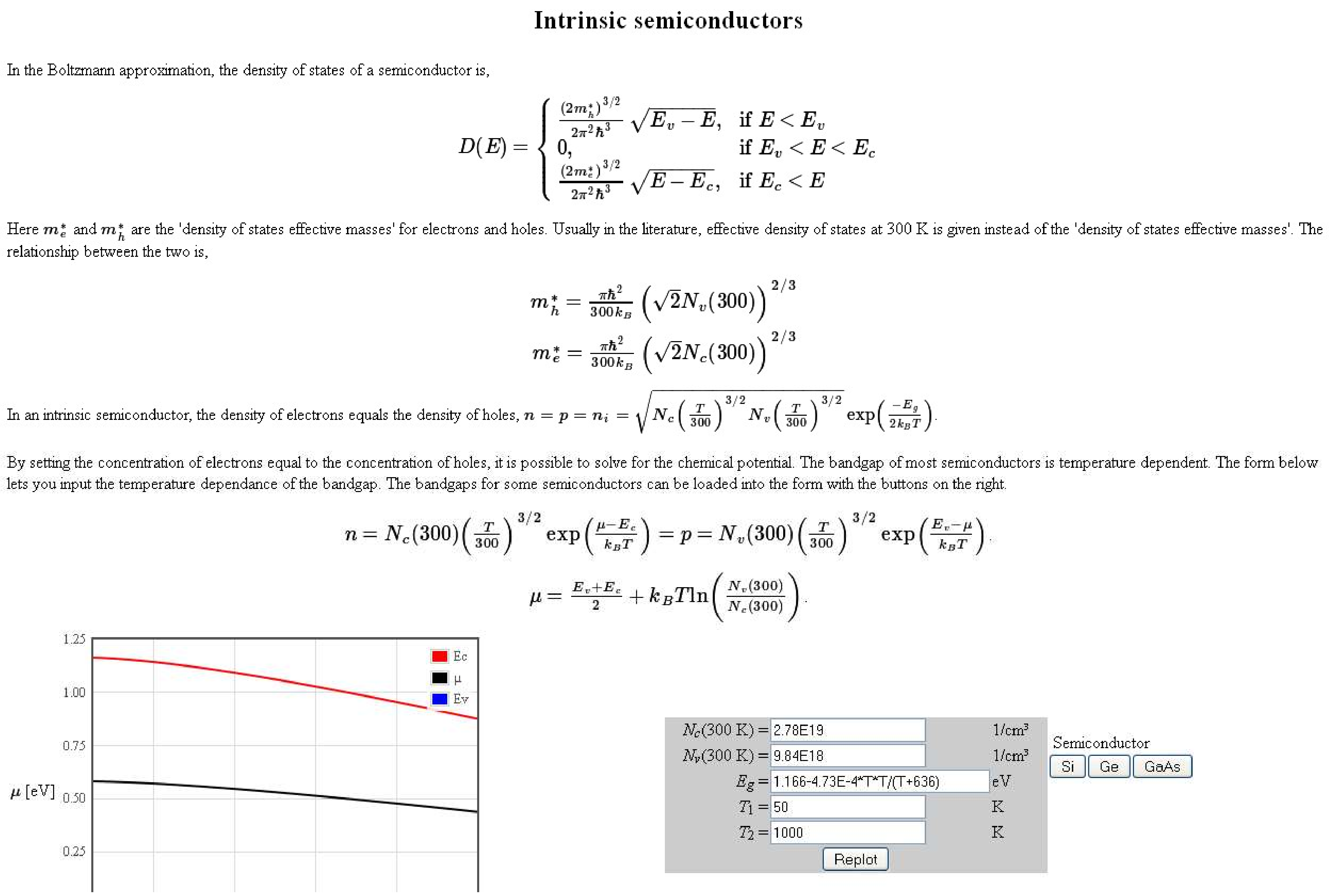
Semiconductors n,k
database InGaAsP Levels Equivalents Bibliografic database

NSM Archive - Physical Properties of Semiconductors

Si	- Silicon	Ge	- Germanium
GaP	- Gallium Phosphide	GaAs	- Gallium Arsenide
InAs	- Indium Arsenide	C	- Diamond
GaSb	- Gallium Antimonide	InSb	- Indium Antimonide
InP	- Indium Phosphide	$GaAs_{1-x}Sb_x$	- Gallium Arsenide Antimonide
$Al_xGa_{1-x}As$	- Aluminium Gallium Arsenide		
AlN	- Aluminium Nitride		
BN	- Boron Nitride		



http://www.matprop.ru/semicond



Intrinsic semiconductors

In the Boltzmann approximation, the density of states of a semiconductor is,

$$D(E) = \begin{cases} \frac{(2m_h^*)^{3/2}}{2\pi^2\hbar^3}\sqrt{E_v - E}, & \text{if } E < E_v \\ 0, & \text{if } E_v < E < E_c \\ \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3}\sqrt{E - E_c}, & \text{if } E_c < E \end{cases}$$

Here m_e^* and m_h^* are the 'density of states effective masses' for electrons and holes. Usually in the literature, effective density of states at 300 K is given instead of the 'density of states effective masses'. The relationship between the two is,

$$m_h^* = \frac{\pi\hbar^2}{300k_B}\left(\sqrt{2}N_v(300)\right)^{2/3}$$

$$m_e^* = \frac{\pi\hbar^2}{300k_B}\left(\sqrt{2}N_c(300)\right)^{2/3}$$

In an intrinsic semiconductor, the density of electrons equals the density of holes, $n = p = n_i = \sqrt{N_c\left(\frac{T}{300}\right)^{3/2}N_v\left(\frac{T}{300}\right)^{3/2}\exp\left(\frac{-E_g}{2k_BT}\right)}$.

By setting the concentration of electrons equal to the concentration of holes, it is possible to solve for the chemical potential. The bandgap of most semiconductors is temperature dependent. The form below lets you input the temperature dependance of the bandgap. The bandgaps for some semiconductors can be loaded into the form with the buttons on the right.

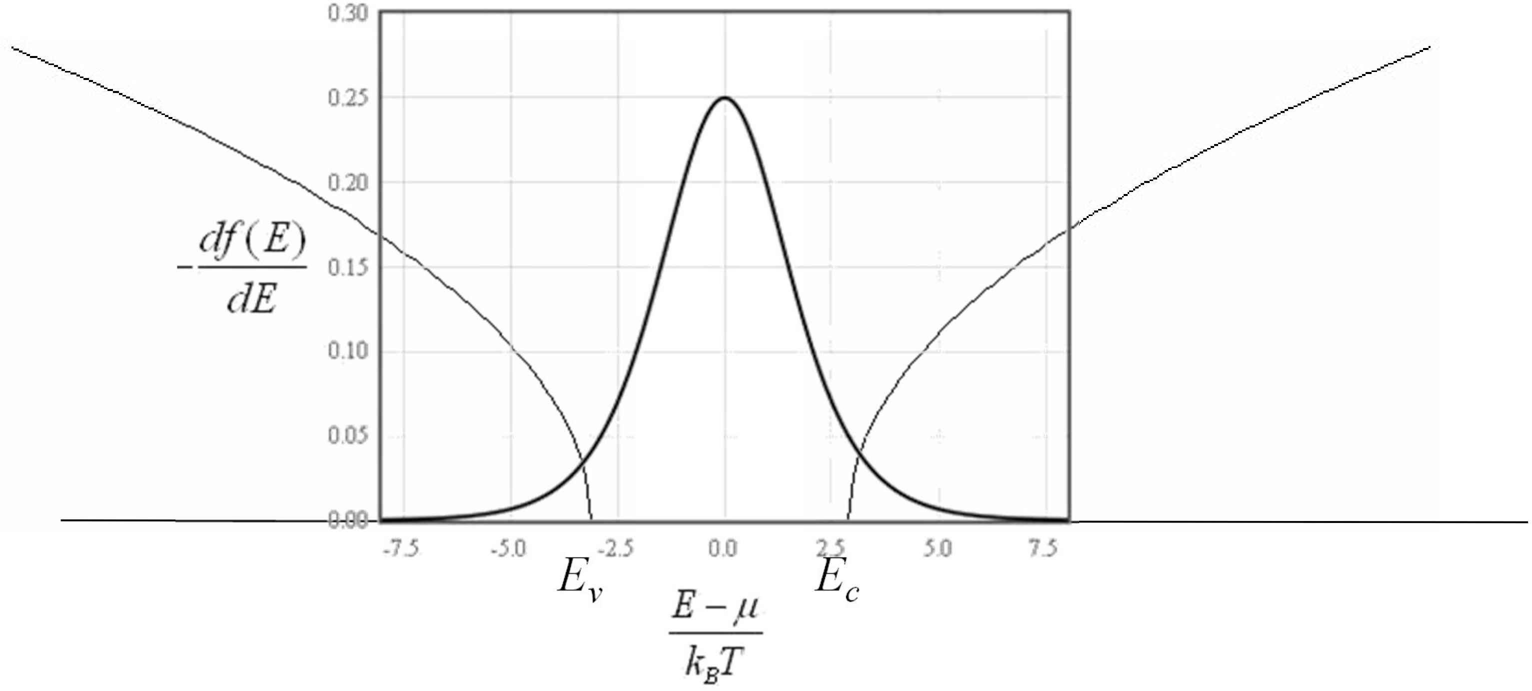
$$n = N_c(300)\left(\frac{T}{300}\right)^{3/2}\exp\left(\frac{\mu - E_c}{k_BT}\right) = p = N_v(300)\left(\frac{T}{300}\right)^{3/2}\exp\left(\frac{E_v - \mu}{k_BT}\right).$$

$$\mu = \frac{E_v + E_c}{2} + k_BT\ln\left(\frac{N_v(300)}{N_c(300)}\right).$$

N_c(300 K) = 2.78E19 1/cm³
N_v(300 K) = 9.84E18 1/cm³
E_g = 1.166-4.73E-4*T*T/(T+636) eV
T_1 = 50 K
T_2 = 1000 K

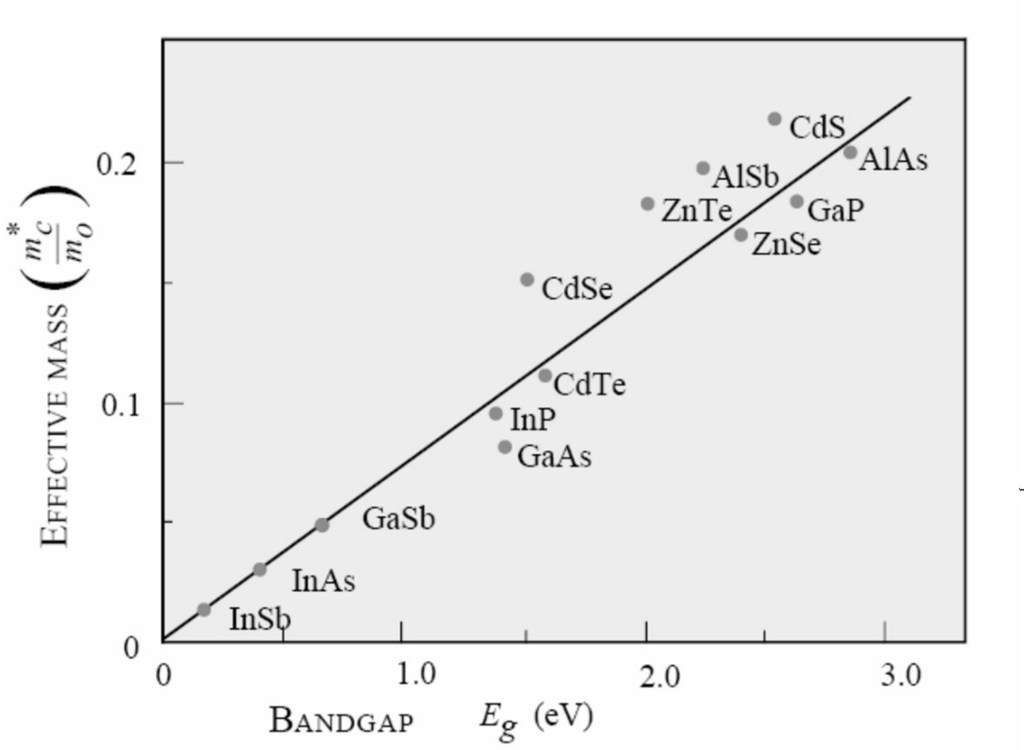
http://lamp.tu-graz.ac.at/~hadley/ss1/semiconductors/intrinsic.php

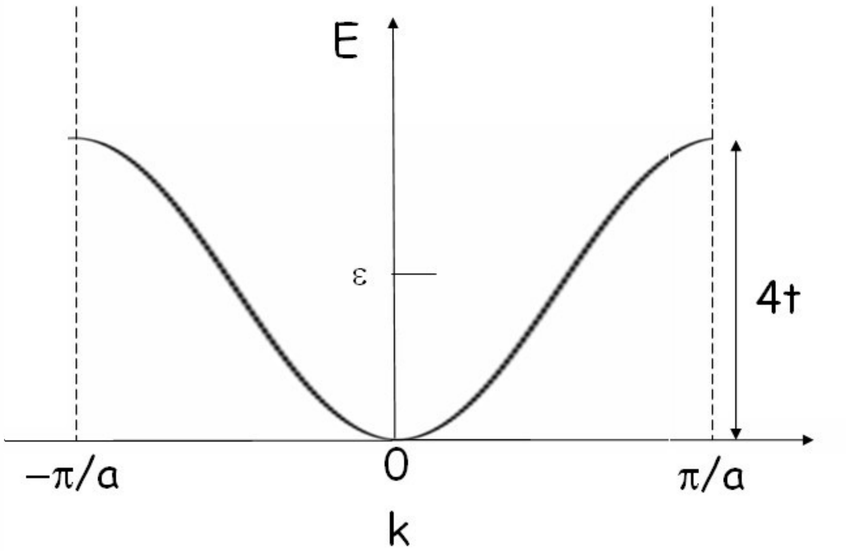
Narrow bandgap semiconductors



Use the programs for metals for small bandgap semiconductors.

Large gap -> large effective mass





$$E_k = \varepsilon - 2t\cos(ka)$$

$$m^* = \frac{\hbar^2}{\frac{d^2E}{dk^2}}$$

$$\frac{d^2E}{dk^2} = 2ta^2$$

$$m^* \square \frac{1}{t}$$

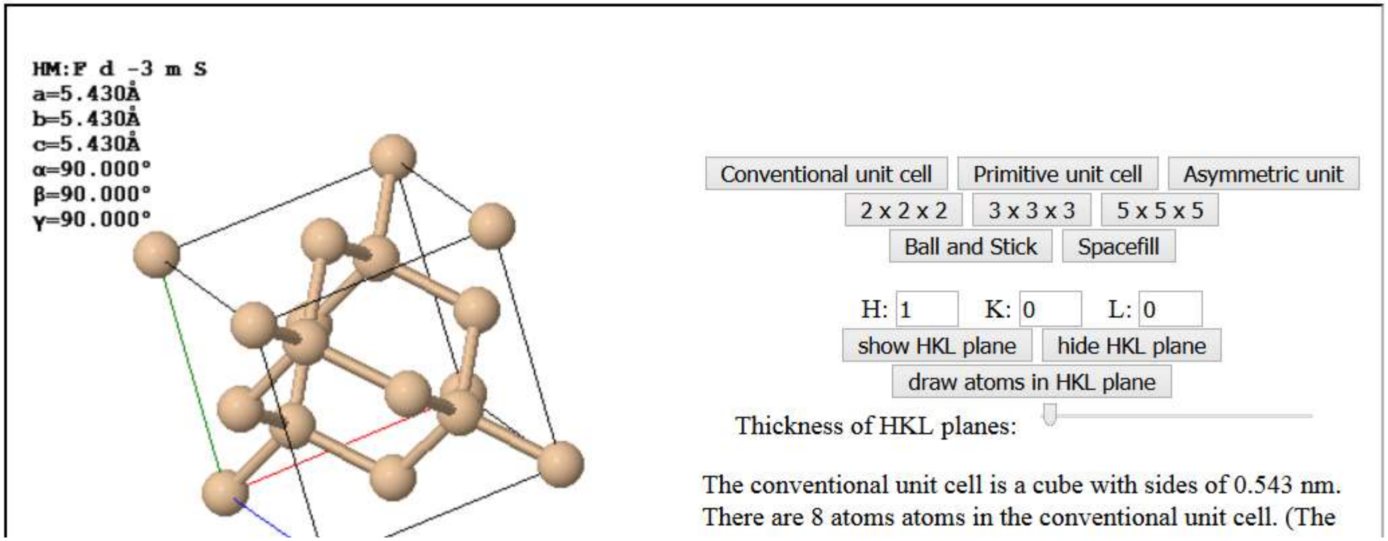
narrow bands -> large effective mass

Silicon

Silicon is the second most common element in the earth's crust and an important semiconducting material.

Structural properties

Crystal structure: Diamond
Bravais lattice: face centered cubic
Space group: 227 (F d -3 m), Strukturbericht: A4, Pearson symbol: cF8
Point group: m3m (O_h) six 2-fold rotations, four 3-fold rotations, three 4-fold rotations, nine mirror planes, inversion
Lattice constant: $a = 0.543$ nm
Atomic weight 28.09
Atomic density $n_{atoms} = 4.995 \times 10^{22}$ 1/cm³
Density $\rho = 2.33$ g/cm³
Density of surface atoms
  (100) 6.78×10^{14} 1/cm²
  (110) 9.59×10^{14} 1/cm²
  (111) 7.83×10^{14} 1/cm²



The conventional unit cell is a cube with sides of 0.543 nm. There are 8 atoms atoms in the conventional unit cell. (The